

Noncommutative analysis and quantum physics

I. Quantities, ensembles and states

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Abstract. In this sequence of papers, noncommutative analysis is used to give a consistent axiomatic approach to a unified conceptual foundation of classical and quantum physics, free of undefined terms.

The present Part I defines the concepts of quantities, ensembles, and states, clarifies the logical relations and operations for them, and shows how they give rise to probabilities and dynamics. The stochastic and the deterministic features of quantum physics are separated in a clear way by consistently distinguishing between ensembles (representing stochastic elements) and states (representing realistic elements).

Ensembles are defined by extending the ‘probability via expectation’ approach of Whittle to noncommuting quantities. This approach carries no connotations of unlimited repeatability; hence it can be applied to unique systems such as the universe. Precise concepts and traditional results about complementarity, uncertainty and nonlocality follow with a minimum of technicalities. Probabilities are introduced in a generality supporting so-called effects (i.e., fuzzy events).

States are defined as partial mappings that provide reference values for certain quantities. An analysis of sharpness properties yields well-known no-go theorems for hidden variables. By dropping the sharpness requirement, hidden variable theories such as Bohmian mechanics can be accommodated, but so-called ensemble states turn out to be a more natural realization of a realistic state concept. The weak law of large numbers explains the emergence of classical properties for macroscopic systems.

Dynamics is introduced via a one-parameter group of automorphisms. A detailed conceptual analysis of the dynamics in terms of Poisson algebras will follow in the second part of this series.

The paper realizes a strong formal implementation of Bohr’s correspondence principle. In all instances, classical and quantum concepts are fully parallel: a single common theory has a classical realization and a quantum realization.

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1 Introduction

“Look,” they say, “here is something new!” But no, it has all happened before, long before we were born.

Kohelet, ca. 250 B.C. [43]

Do not imagine, any more than I can bring myself to imagine, that I should be right in undertaking so great and difficult a task. Remembering what I said at first about probability, I will do my best to give as probable an explanation as any other – or rather, more probable; and I will first go back to the beginning and try to speak of each thing and of all.

Plato, ca. 367 B.C. [64]

This paper is the first one of a series of papers designed to give a mathematically elementary and philosophically consistent axiomatic foundation of modern theoretical physics, free of undefined terms. It is an attempt to reconsider, from the point of view of noncommutative analysis, HILBERT’s [33] sixth problem, the *axiomatization of theoretical physics*. (It is an attempt only since at the present stage of development, I have not yet tried to achieve full mathematical rigor everywhere. However, the present Part I is completely rigorous, and in later parts the few places where the standard of rigor is relaxed will be explicitly mentioned.)

The purpose is to provide precise mathematical concepts that match all concepts that physicists use to describe their experiments and their theory, in sufficiently close correspondence to reproduce at least that part of physics that is amenable to numerical verification.

One of the basic premises of this work is that the split between classical physics and quantum physics should be as small as possible. Except in the examples, the formalism never distinguishes between the classical and the quantum situation. Thus it can be considered as a consequent implementation of BOHR’s *correspondence principle*. This also has didactical advantages for teaching: Students can be trained to be acquainted with the formalism by means of intuitive, primarily classical examples at first. Later, without having to unlearn anything, they can apply the same formalism to quantum phenomena.

The present Part I is concerned with giving (more carefully than usual, and without reference to measurement) a concise foundation by defining the concepts of quantities, ensembles, and states, clarifying the logical relations and operations for them, and showing how they give rise to the traditional pos-

tulates of quantum mechanics, including probabilities and dynamics.

The stochastic and the deterministic features of quantum physics are separated in a clear way by consistently distinguishing between ensembles (representing stochastic elements) and states (representing realistic elements).

Most of what is done here is common wisdom in quantum mechanics; see, e.g., JAMMER [39, 40], JAUCH [41], MESSIAH [49], VON NEUMANN [54].

However, the new interpretation slightly shifts the meaning of the concept of a state, fixing it in a way that allows to embed and analyze different interpretations of the quantum mechanical formalism, including both orthodox views such as the Copenhagen interpretation and hidden-variable theories such as Bohmian mechanics.

To motivate the conceptual foundation and to place it into context, I found it useful to embed the formalism into my philosophy of physics, while *strictly separating the mathematics by using a formal definition-example-theorem-proof exposition style*. Though I present my view generally without using subjunctive formulations or qualifying phrases, I do not claim that this is the only way to understand physics. However, I did attempt to integrate different points of view. And I believe that my philosophical view is consistent with the mathematical formalism of quantum mechanics and accommodates naturally a number of puzzling questions about the nature of the world.

The stochastic contents of quantum theory is determined by the restrictions noncommutativity places upon the preparation of experiments. Since the information going into the preparation is always extrapolated from finitely many observations in the past, it can only be described in a statistical way, i.e., by ensembles.

Ensembles are defined by extending to noncommuting quantities WHITTLE's [77] elegant expectation approach to classical probability theory. This approach carries no connotations of unlimited repeatability; hence it can be applied to unique systems such as the universe. The weak law of large numbers relates abstract ensembles and concrete mean values over many instances of quantities with the same stochastic behavior within a single system.

Precise concepts and traditional results about complementarity, uncertainty and nonlocality follow with a minimum of technicalities. In particular, non-local correlations predicted by BELL [2] and first detected by ASPECT [1] are shown to be already consequences of the nature of quantum mechanical ensembles and do not depend on hidden variables or on counterfactual reasoning.

The concept of probability itself is derived from that of an ensemble by means

of a formula motivated from classical ensembles that can be described as a finite weighted mean of properties of finitely many elementary events. Probabilities are introduced in a generality supporting so-called effects, a sort of fuzzy events (related to POV measures that play a significant role in measurement theory; see BUSCH et al. [8, 9], DAVIES [14], PERES [62]). The weak law of large numbers provides the relation to the frequency interpretation of probability. As a special case of the definition, one gets without any effort the well-known squared probability amplitude formula for transition probabilities.

States are defined as partial mappings that provide objective reference values for certain quantities. Sharpness of quantities is defined in terms of laws for the reference values, in particular the squaring law that requires the value of a squared sharp quantity f to be equal to the squared value of f . It is shown that the values of sharp quantities must belong to their spectrum, and that requiring all quantities to be sharp produces contradictions over Hilbert spaces of dimension > 3 . This is related to well-known no-go theorems for hidden variables. (However, recent constructive results by CLIFTON & KENT [13] show that in the finite-dimensional case there are states with a dense set of sharp quantities.)

An analysis of a well-known macroscopic reference value, the center of mass, leads us to reject the sharpness requirement. Without universal sharpness, hidden variable theories such as Bohmian mechanics (BOHM [6]; cf. HOLLAND [35]) can be accommodated. However, the Bohmian states violate monotony, and so-called ensemble states turn out to be a more natural realization of a realistic state concept.

With ensemble states, quantum objects are intrinsically extended, real objects; e.g., the reference radius of a hydrogen atom in the ground state is 1.5 times the Bohr radius. Moreover, in ensemble states, the weak law of large numbers explains the emergence of classical properties for macroscopic systems.

Thus ensemble states provide an elegant solution to the reality problem, confirming the insistence of the orthodox Copenhagen interpretation on that there is nothing but ensembles, while avoiding their elusive reality picture.

Finally, it is outlined how dynamical properties fit into the present setting. Dynamics is introduced via a one-parameter group of automorphisms. A detailed conceptual analysis of the dynamics in terms of a differential calculus based on Poisson algebras will follow in the second part of this series.

Subsequent parts of this sequence of papers will present the calculus of in-

tegration and its application to equilibrium thermodynamics, a theory of measurement, a relativistic covariant Hamiltonian multiparticle theory, and its application to nonequilibrium thermodynamics and field theory.

As in this first paper, each topic will be presented in a uniform way, classical and quantum versions being only special cases of a single theory.

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2 Quantities

Only love transcends our limitations. In contrast, our predictions can fail, our communication can fail, and our knowledge can fail. For our knowledge is patchwork, and our predictive power is limited. But when perfection comes, all patchwork will disappear.

St. Paul, ca. 57 A.D. [58]

But you [God] have ordered everything with measure, number and weight.

Wisdom 11:20, ca. 50 B.C.

All our scientific knowledge is based on past observation, and only gives rise to conjectures about the future. Mathematical consistency requires that our choices are constrained by some formal laws. When we want to predict something, the true answer depends on knowledge we do not have. We can calculate at best approximations whose accuracy can be estimated using statistical techniques (assuming that the quality of our models is good).

This implies that we must distinguish between *quantities* (formal concepts of what can possibly be measured or calculated) and *numbers* (the results of measurements and calculations themselves); those quantities that are constant by the nature of the concept considered behave just like numbers.

Physicists are used to calculating with quantities that they may add and multiply without restrictions; if the quantities are complex, the complex conjugate can also be formed. It must also be possible to compare quantities, at least in certain cases.

Therefore we take as primitive objects of our treatment a set \mathbb{E} of quantities, such that the sum and the product of quantities is again a quantity, and there is an operation generalizing complex conjugation. Moreover, we assume that

there is an ordering relation that allows us to compare two quantities.

Operations on quantities and their comparison are required to satisfy a few simple rules; they are called **axioms** since we take them as a formal starting point without making any further demands on the nature of the symbols we are using. Our axioms are motivated by the wish to be as general as possible while still preserving the ability to manipulate quantities in the manner familiar from matrix algebra. (Similar axioms for quantities have been proposed, e.g., by DIRAC [15].)

2.1 Definition.

(i) \mathbb{E} denotes a set whose elements are called **quantities**. For any two quantities $f, g \in \mathbb{E}$, the **sum** $f + g$, the **product** fg , and the **conjugate** f^* are also quantities. It is also specified for which pairs of quantities the relation $f \geq g$ holds.

The following axioms (Q1)–(Q8) are assumed to hold for all complex numbers $\alpha \in \mathbb{C}$ and all quantities $f, g, h \in \mathbb{E}$.

(Q1) $\mathbb{C} \subseteq \mathbb{E}$, i.e., complex numbers are special quantities, where addition, multiplication and conjugation have their traditional meaning.

(Q2) $(fg)h = f(gh)$, $\alpha f = f\alpha$, $0f = 0$, $1f = f$.

(Q3) $(f + g) + h = f + (g + h)$, $f(g + h) = fg + fh$, $f + 0 = f$.

(Q4) $f^{**} = f$, $(fg)^* = g^*f^*$, $(f + g)^* = f^* + g^*$.

(Q5) $f^*f = 0 \Rightarrow f = 0$.

(Q6) \geq is a partial order, i.e., it is reflexive ($f \geq f$), antisymmetric ($f \geq g \geq f \Rightarrow f = g$) and transitive ($f \geq g \geq h \Rightarrow f \geq h$).

(Q7) $f \geq g \Rightarrow f + h \geq g + h$.

(Q8) $f \geq 0 \Rightarrow f = f^*$ and $g^*fg \geq 0$.

(Q9) $1 \geq 0$.

If (Q1)–(Q9) are satisfied we say that \mathbb{E} is a **Q-algebra**.

(ii) We introduce the traditional notation

$$\begin{aligned} f \leq g &:= g \geq f, \\ -f &:= (-1)f, \quad f - g := f + (-g), \quad [f, g] := fg - gf, \\ f^0 &:= 1, \quad f^l := f^{l-1}f \quad (l = 1, 2, \dots), \\ \operatorname{Re} f &= \frac{1}{2}(f + f^*), \quad \operatorname{Im} f = \frac{1}{2i}(f - f^*), \\ \|f\| &= \inf\{\alpha \in \mathbb{R} \mid f^*f \leq \alpha^2, \alpha \geq 0\}. \end{aligned}$$

(The infimum of the empty set is taken to be ∞ .) $[f, g]$ is called the **commutator** of f and g , $\operatorname{Re} f$, $\operatorname{Im} f$ and $\|f\|$ are referred to as the **real part**, the **imaginary part**, and the **(spectral) norm** of f , respectively. The **uniform topology** is the topology induced on \mathbb{E} by declaring a set E open if it contains a ball $\{f \in \mathbb{E} \mid \|f\| < \varepsilon\}$ for some $\varepsilon > 0$.

(iii) A quantity $f \in \mathbb{E}$ is called **bounded** if $\|f\| < \infty$, **Hermitian** if $f^* = f$, and **normal** if $[f, f^*] = 0$. More generally, a set F of quantities is called **normal** if all its quantities commute with each other and with their conjugates.

Note that every Hermitian quantity (and in a commutative algebra, every quantity) is normal. Physical observables will be among the normal quantities, but until we define (in a later part of this sequence of papers) what it means to ‘observe’ a quantity we avoid talking about observables.

2.2 Examples.

(i) The commutative algebra $\mathbb{E} = \mathbb{C}^n$ with pointwise multiplication and componentwise inequalities is a Q-algebra, if vectors with constant entries α are identified with $\alpha \in \mathbb{C}$. This Q-algebra describes properties of n classical elementary events; cf. Example 4.2(i).

(ii) $\mathbb{E} = \mathbb{C}^{n \times n}$ is a Q-algebra if complex numbers are identified with the scalar multiples of the identity matrix, and $f \geq g$ iff $f - g$ is Hermitian and positive semidefinite. This Q-algebra describes quantum systems with n levels. For $n = 2$, it also describes a single spin, or a qubit.

(iii) The algebra of all complex-valued functions on a set Ω , with pointwise multiplication and pointwise inequalities is a Q-algebra. Suitable subalgebras of such algebras describe classical probability theory – cf. Example 7.3(i) – and classical mechanics – cf. Example 8.2(i). In the latter case, Ω is the phase space of the system considered.

(iv) The algebra of bounded linear operators on a Hilbert space \mathbb{H} , with $f \geq g$ iff $f - g$ is Hermitian and positive semidefinite, is a Q-algebra. They (or the more general C^* -algebras and von Neumann algebras) are frequently taken as the basis of nonrelativistic quantum mechanics.

(v) The algebra of continuous linear operators on the Schwartz space $\mathcal{S}(\Omega_{qu})$ of rapidly decaying functions on a manifold Ω_{qu} is a Q-algebra. It also allows the discussion of unbounded quantities. In quantum physics, Ω_{qu} is the configuration space of the system.

Note that physicist generally need to work with unbounded quantities, while much of the discussion on foundations takes the more restricted Hilbert space

point of view. The theory presented here is formulated in a way to take care of unbounded quantities, while in our examples, we select the point of view as deemed profitable.

We shall see that, for the general, qualitative aspects of the theory there is no need to know any details of how to actually perform calculations with quantities; this is only needed if one wants to calculate specific properties for specific systems. In this respect, the situation is quite similar to the traditional axiomatic treatment of real numbers: The axioms specify the permitted ways to handle formulas involving these numbers; and this is enough to derive calculus, say, without the need to specify either what real numbers *are* or algorithmic rules for addition, multiplication and division. Of course, the latter are needed when one wants to do specific calculations but not while one tries to get insight into a problem. And as the development of pocket calculators has shown, the capacity for understanding theory and that for knowing the best ways of calculation need not even reside in the same person.

Note that we assume commutativity only between numbers and quantities. However, general commutativity of the addition is a consequence of our other assumptions. We prove this together with some other useful relations.

2.3 Proposition. *For all quantities $f, g, h \in \mathbb{E}$ and $\lambda \in \mathbb{C}$,*

$$(f + g)h = fh + gh, \quad f - f = 0, \quad f + g = g + f \quad (1)$$

$$[f, f^*] = -2i[\operatorname{Re} f, \operatorname{Im} f], \quad (2)$$

$$f^* f \geq 0, \quad ff^* \geq 0. \quad (3)$$

$$f^* f \leq 0 \quad \Rightarrow \quad \|f\| = 0 \quad \Rightarrow \quad f = 0, \quad (4)$$

$$f \leq g \quad \Rightarrow \quad h^* f h \leq h^* g h, \quad |\lambda|f \leq |\lambda|g, \quad (5)$$

$$f^* g + g^* f \leq 2\|f\| \|g\|, \quad (6)$$

$$\|\lambda f\| = |\lambda|\|f\|, \quad \|f \pm g\| \leq \|f\| \pm \|g\|, \quad (7)$$

$$\|fg\| \leq \|f\| \|g\|. \quad (8)$$

Proof. The right distributive law follows from

$$\begin{aligned} (f + g)h &= ((f + g)h)^{**} = (h^*(f + g)^*)^* = (h^*(f^* + g^*))^* \\ &= (h^*f^* + h^*g^*)^* = (h^*f^*)^* + (h^*g^*)^* \\ &= f^{**}h^{**} + g^{**}h^{**} = fh + gh. \end{aligned}$$

It implies $f - f = 1f - 1f = (1 - 1)f = 0f = 0$. From this, we may deduce that addition is commutative, as follows. The quantity $h := -f + g$ satisfies

$$-h = (-1)((-1)f + g) = (-1)(-1)f + (-1)g = f - g,$$

and we have

$$f + g = f + (h - h) + g = (f + h) + (-h + g) = (f - f + g) + (f - g + g) = g + f.$$

This proves (1). If $u = \operatorname{Re} f$, $v = \operatorname{Im} f$ then $u^* = u, v^* = v$ and $f = u + iv, f^* = u - iv$. Hence

$$[f, f^*] = (u + iv)(u - iv) - (u - iv)(u + iv) = 2i(vu - uv) = -2i[\operatorname{Re} f, \operatorname{Im} f],$$

giving (2). (3)–(5) follow directly from (Q7) – (Q9). Now let $\alpha = \|f\|$, $\beta = \|g\|$. Then $f^*f \leq \alpha^2$ and $g^*g \leq \beta^2$. Since

$$\begin{aligned} 0 \leq (\beta f - \alpha g)^*(\beta f - \alpha g) &= \beta^2 f^*f - \alpha\beta(f^*g + g^*f) + \alpha^2 g^*g \\ &\leq \beta^2 \alpha^2 \pm \alpha\beta(f^*g + g^*f) + \alpha^2 g^*g, \end{aligned}$$

$f^*g + g^*f \leq 2\alpha\beta$ if $\alpha\beta \neq 0$, and for $\alpha\beta = 0$, the same follows from (4). Therefore (6) holds. The first half of (7) is trivial, and the second half follows for the plus sign from

$$(f + g)^*(f + g) = f^*f + f^*g + g^*f + g^*g \leq \alpha^2 + 2\alpha\beta + \beta^2 = (\alpha + \beta)^2,$$

and then for the minus sign from the first half. Finally, by (5),

$$(fg)^*(fg) = g^*f^*fg \leq g^*\alpha^2g = \alpha^2g^*g \leq \alpha^2\beta^2.$$

This implies (8). □

2.4 Corollary.

(i) Among the complex numbers, precisely the nonnegative real numbers λ satisfy $\lambda \geq 0$.

(ii) For all $f \in \mathbb{E}$, $\operatorname{Re} f$ and $\operatorname{Im} f$ are Hermitian. f is Hermitian iff $f = \operatorname{Re} f$ iff $\operatorname{Im} f = 0$. If f, g are commuting Hermitian quantities then fg is Hermitian, too.

(iii) f is normal iff $[\operatorname{Re} f, \operatorname{Im} f] = 0$.

Proof. (i) If λ is a nonnegative real number then $\lambda = f^*f \geq 0$ with $f = \sqrt{\lambda}$. If λ is a negative real number then $\lambda = -f^*f \leq 0$ with $f = \sqrt{-\lambda}$, and by

antisymmetry, $\lambda \geq 0$ is impossible. If λ is a nonreal number then $\lambda \neq \lambda^*$ and $\lambda \geq 0$ is impossible by (Q8).

The first two assertions of (ii) are trivial, and the third holds since $(fg)^* = g^*f^* = gf = fg$ if f, g are Hermitian and commute.

(iii) follows from (2). \square

Thus, in conventional terminology (see, e.g., RICKART [66]), \mathbb{E} is a **partially ordered nondegenerate *-algebra with unity**, but not necessarily with a commutative multiplication.

2.5 Remark. In the realizations of the axioms I know of, e.g., in C^* -algebras (RICKART [66]), we also have the relations

$$\|f^*\| = \|f\|, \quad \|f^*f\| = \|f\|^2,$$

and

$$0 \leq f \leq g \quad \Rightarrow \quad f^2 \leq g^2,$$

but I have not been able to prove these from the present axioms, and they were not needed to develop the theory.

As the example $\mathbb{E} = \mathbb{C}^{n \times n}$ shows, \mathbb{E} may have zero divisors, and not every nonzero quantity need have an inverse. Therefore, in the manipulation of formulas, precisely the same precautions must be taken as in ordinary matrix algebra.

3 Complementarity

You cannot have the penny and the cake.
Proverb

The lack of commutativity gives rise to the phenomenon of complementarity, expressed by inequalities that demonstrate the danger of simply thinking of quantities in terms of numbers.

3.1 Definition. Two Hermitian quantities f, g are called **complementary** if there is a real number $\gamma > 0$ such that

$$(f - x)^2 + (g - y)^2 \geq \gamma^2 \quad \text{for all } x, y \in \mathbb{R}. \tag{9}$$

3.2 Examples.

(i) The \mathbb{Q} -algebra of all complex-valued functions on a set Ω contains no complementary pair of quantities. Indeed, setting $x = f(\omega)$, $y = g(\omega)$ in (9), we find $0 \geq \gamma^2$, contradicting complementarity.

Thus complementarity captures the phenomenon where two quantities do not have simultaneous sharp classical ‘values’. (See also Section 8.)

(ii) $\mathbb{C}^{2 \times 2}$ contains a complementary pair of quantities. Indeed, the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (10)$$

are complementary; see Proposition 3.3(i) below.

(iii) The algebra of bounded linear operators on a Hilbert space of dimension > 1 contains a complementary pair of quantities, since it contains many subalgebras isomorphic to $\mathbb{C}^{2 \times 2}$.

(iv) In the algebra of all linear operators on the Schwartz space $\mathcal{S}(\mathbb{R})$, **position** q , defined by

$$(qf)(x) = xf(x),$$

and **momentum** p , defined by

$$(pf)(x) = -i\hbar f'(x),$$

where $\hbar > 0$ is Planck’s constant, are complementary. Since q and p are Hermitian, this follows from the easily verified **canonical commutation relation**

$$[q, p] = i\hbar \quad (11)$$

and Proposition 3.3(ii) below.

3.3 Proposition.

(i) The Pauli matrices (10) satisfy

$$(\sigma_1 - s_1)^2 + (\sigma_3 - s_3)^2 \geq 1 \quad \text{for all } s_1, s_3 \in \mathbb{R}. \quad (12)$$

(ii) Let p, q be Hermitian quantities satisfying $[q, p] = i\hbar$. Then, for any $k, x \in \mathbb{R}$ and any positive $\Delta p, \Delta q \in \mathbb{R}$,

$$\left(\frac{p - k}{\Delta p}\right)^2 + \left(\frac{q - x}{\Delta q}\right)^2 \geq \frac{\hbar}{\Delta p \Delta q}. \quad (13)$$

Proof. (i) A simple calculation gives

$$(\sigma_1 - s_1)^2 + (\sigma_3 - s_3)^2 - 1 = \begin{pmatrix} s_1^2 + (1 - s_3)^2 & -2s_1 \\ -2s_1 & s_1^2 + (1 + s_3)^2 \end{pmatrix} \geq 0,$$

since the diagonal is nonnegative and the determinant is $(s_1^2 + s_3^2 - 1)^2 \geq 0$.

(ii) The quantities $f = (q - x)/\Delta q$ and $g = (p - k)/\Delta p$ are Hermitian and satisfy $[f, g] = [q, p]/\Delta q \Delta p = i\kappa$ where $\kappa = \hbar/\Delta q \Delta p$. Now (13) follows from

$$0 \leq (f + ig)^*(f + ig) = f^2 + g^2 + i[f, g] = f^2 + g^2 - \kappa.$$

□

The complementarity of position and momentum expressed by (22) is the deeper reason for the Heisenberg uncertainty relation discussed later in (22) and (23).

3.4 Theorem. *In $\mathbb{C}^{n \times n}$, two complementary quantities cannot commute.*

Proof. Any two commuting quantities f, g have a common eigenvector ψ . If $f\psi = x\psi$ and $g\psi = y\psi$ then $\psi^*((f - x)^2 + (g - y)^2)\psi = 0$, whereas (9) implies

$$\psi^*(f - x)^2 + (g - y)^2\psi \geq \gamma^2 \psi^* \psi > 0.$$

Thus f, g cannot be complementary. □

I have not been able to decide whether complementary quantities can possibly commute. (It is impossible when there is a joint spectral resolution.)

4 Ensembles

We may assume that words are akin to the matter which they describe; when they relate to the lasting and permanent and intelligible, they ought to be lasting and unalterable, and, as far as their nature allows, irrefutable and immovable – nothing less. But when they express only the copy or likeness and not the eternal things themselves, they need only be likely and analogous to the real words. As being is to becoming, so is truth to belief.

Plato, ca. 367 B.C. [64]

The stochastic nature of quantum mechanics is usually discussed in terms of *probabilities*. However, from a strictly logical point of view, this has the

drawback that one gets into conflict with the traditional foundation of probability theory by KOLMOGOROV [45], which does not extend to the noncommutative case. Mathematical physicists (see, e.g., PARTHASARATHY [57], MEYER [51]) developed a far reaching quantum probability calculus based on Hilbert space theory. But their approach is highly formal, drawing its motivation from analogies to the classical case rather than from the common operational meaning.

WHITTLE [77] presents a much less known alternative approach to classical probability theory, equivalent to that of Kolmogorov, that treats *expectation* as the basic concept and derives probability from axioms for the expectation. (See the discussion in [77, Section 3.4] why, for historical reasons, this has remained a minority approach.)

The approach via expectations is easy to motivate, leads quickly to interesting results, and extends without much trouble to the quantum world, yielding the ensembles (‘mixed states’) of traditional quantum physics. As we shall see, explicit probabilities enter only at a very late stage of the development.

A significant advantage of the expectation approach compared with the probability approach is that it is intuitively more removed from connotations of ‘unlimited repeatability’. Hence it can be naturally used for *unique* systems such as the set of all natural globular proteins (cf., e.g., NEUMAIER [53]), the climate of the earth, or the universe, and to deterministic, pseudo-random behavior such as rounding errors in floating point computations (cf., e.g., HIGHAM [32, Section 2.6]), once these have enough complexity to exhibit finite *internal* repetitivity to which the weak law of large numbers (Theorem 4.4 below) may be applied.

The axioms we shall require for meaningful expectations are those trivially satisfied for weighted averages of a finite ensemble of observations. While this motivates the form of the axioms and the name ‘ensemble’ attached to the concept, there is no need at all to interpret expectation as an average; this is the case only in certain classical situations. In general, ensembles are simply a way to consistently organize structured data obtained by some process of observation.

For the purpose of statistical analysis and prediction, it is completely irrelevant what this process of observation entails. What matters is only that for certain quantities observed values are available that can be compared with their expectations. The expectation of a quantity f is simply a value near which, based on the theory, we should expect an observed value for f . At the same time, the standard deviation serves as a measure of the amount to which we should expect this nearness to deviate from exactness.

For science, however, it is of utmost importance to have well-defined protocols that specify what are valid observations. Such standardized protocols guarantee that the observations are repeatable and hence objective. On the other hand, these protocols require a level of description not appropriate for the foundations of a discipline. Therefore, at the present fundamental level of exposition, observed values are undefined, and not yet part of the formal development. In physics, they need a theory of measurement, which will be discussed in a later part of this sequence of papers.

4.1 Definition.

(i) An **ensemble** is a mapping $\bar{\cdot}$ that assigns to each quantity $f \in \mathbb{E}$ its **expectation** $\bar{f} =: \langle f \rangle \in \mathbb{C}$ such that for all $f, g \in \mathbb{E}$, $\alpha \in \mathbb{C}$,

$$(E1) \quad \langle 1 \rangle = 1, \quad \langle f^* \rangle = \langle f \rangle^*, \quad \langle f + g \rangle = \langle f \rangle + \langle g \rangle,$$

$$(E2) \quad \langle \alpha f \rangle = \alpha \langle f \rangle,$$

$$(E3) \quad \text{If } f \geq 0 \text{ then } \langle f \rangle \geq 0,$$

$$(E4) \quad \text{If } f_l \in \mathbb{E}, f_l \downarrow 0 \text{ then } \inf \langle f_l \rangle = 0.$$

Here $f_l \downarrow 0$ means that the f_l converge almost everywhere to 0 and $f_{l+1} \leq f_l$ for all l .

(ii) The number

$$\text{cov}(f, g) := \text{Re}(\langle (f - \bar{f})^*(g - \bar{g}) \rangle)$$

is called the **covariance** of $f, g \in \mathbb{E}$. Two quantities f, g are called **correlated** if $\text{cov}(f, g) \neq 0$, and **uncorrelated** otherwise.

(iii) The number

$$\sigma(f) := \sqrt{\text{cov}(f, f)}$$

is called the **uncertainty** or **standard deviation** of $f \in \mathbb{E}$ in the ensemble $\langle \cdot \rangle$.

(We shall not use axiom (E4) in this paper and therefore defer technicalities about almost everywhere convergence to a more detailed treatment in a later part of this sequence of papers).

This definition generalizes the expectation axioms of WHITTLE [77, Section 2.2] for classical probability theory and the definitions of elementary classical statistics. Note that (E3) ensures that $\sigma(f)$ is a nonnegative real number that vanishes if f is a constant quantity (i.e., a complex number).

4.2 Examples.

(i) **Finite probability theory.** In the commutative Q-algebra $\mathbb{E} = \mathbb{C}^n$ with pointwise multiplication and componentwise inequalities, every linear

functional on \mathbb{E} , and in particular every ensemble, has the form

$$\langle f \rangle = \sum_{k=1}^n p_k f_k \quad (14)$$

for certain weights p_k . The ensemble axioms hold precisely when the p_k are nonnegative and add up to one; thus $\langle f \rangle$ is a weighted average, and the weights have the intuitive meaning of ‘probabilities’.

Note that the weights can be recovered from the expectation by means of the formula $p_k = \langle e_k \rangle$, where e_k is the unit vector with a one in component k .

(ii) **Quantum mechanical ensembles.** In the Q-algebra \mathbb{E} of bounded linear operators on a Hilbert space \mathbb{H} , quantum mechanics describes a **pure ensemble** (traditionally called a ‘pure state’, but we shall reserve the name ‘state’ for a concept defined in Section 8) by the expectation

$$\langle f \rangle := \psi^* f \psi,$$

where $\psi \in \mathbb{H}$ is a unit vector. And quantum thermodynamics describes an **equilibrium ensemble** by the expectation

$$\langle f \rangle := \text{tr } e^{-S/\bar{k}} f,$$

where $\bar{k} > 0$ is the **Boltzmann constant**, and S is a Hermitian quantity with $\text{tr } e^{-S/\bar{k}} = 1$ called the **entropy** whose spectrum is discrete and bounded below. In both cases, the ensemble axioms are easily verified.

4.3 Proposition. *For any ensemble,*

$$(i) \quad f \leq g \quad \Rightarrow \quad \langle f \rangle \leq \langle g \rangle.$$

$$(iii) \quad \text{For } f, g \in \mathbb{E},$$

$$\text{cov}(f, g) = \text{Re}(\langle f^* g \rangle - \langle f \rangle^* \langle g \rangle),$$

$$\langle f^* f \rangle = \langle f \rangle^* \langle f \rangle + \sigma(f)^2,$$

$$|\langle f \rangle| \leq \sqrt{\langle f^* f \rangle}.$$

$$(iii) \quad \text{If } f \text{ is Hermitian then } \bar{f} = \langle f \rangle \text{ is real and}$$

$$\sigma(f) = \sqrt{\langle (f - \bar{f})^2 \rangle} = \sqrt{\langle f^2 \rangle - \langle f \rangle^2}.$$

$$(iv) \quad \text{Two commuting Hermitian quantities } f, g \text{ are uncorrelated iff}$$

$$\langle fg \rangle = \langle f \rangle \langle g \rangle.$$

Proof. (i) follows from (E1) and (E3).

(ii) The first formula holds since

$$\langle (f - \bar{f})^*(g - \bar{g}) \rangle = \langle f^*g \rangle - \bar{f}^*\langle g \rangle - \langle f \rangle^*\bar{g} + \bar{f}^*\bar{g} = \langle f^*g \rangle - \langle f \rangle^*\langle g \rangle.$$

The second formula follows for $g = f$, using (E1), and the third formula is an immediate consequence.

(iii) follows from (E1) and (ii).

(iv) If f, g are Hermitian and commute the fg is Hermitian by Corollary 2.4(ii), hence $\langle fg \rangle$ is real. By (iii), $\text{cov}(f, g) = \langle fg \rangle - \langle f \rangle \langle g \rangle$, and the assertion follows. □

Fundamental for the practical use of ensembles, and basic to statistical mechanics, is the **weak law of large numbers**:

4.4 Theorem. *For a family of quantities f_l ($l = 1, \dots, N$) with constant expectation $\langle f_l \rangle = \mu$, the **mean value***

$$\bar{f} := \frac{1}{N} \sum_{l=1}^N f_l$$

satisfies

$$\langle \bar{f} \rangle = \mu.$$

If, in addition, the f_l are uncorrelated and have constant standard deviation $\sigma(f_l) = \sigma$ then

$$\sigma(\bar{f}) = \sigma/\sqrt{N} \tag{15}$$

becomes arbitrarily small as N becomes sufficiently large.

Proof. We have

$$\langle \bar{f} \rangle = \frac{1}{N} (\langle f_1 \rangle + \dots + \langle f_N \rangle) = \frac{1}{N} (\mu + \dots + \mu) = \mu$$

and

$$\bar{f}^* \bar{f} = \frac{1}{N^2} \left(\sum_j f_j \right)^* \left(\sum_k f_k \right) = N^{-2} \sum_{j,k} f_j^* f_k.$$

Now

$$\langle f_j^* f_j \rangle = \langle f_j \rangle^* \langle f_j \rangle + \sigma(f_j)^2 = |\mu|^2 + \sigma^2$$

and, if the f_l are uncorrelated, for $j \neq k$,

$$\langle f_j^* f_k + f_k^* f_j \rangle = 2 \operatorname{Re} \langle f_j^* f_k \rangle = 2 \operatorname{Re} \langle f_j \rangle^* \langle f_k \rangle = 2 \operatorname{Re} \mu^* \mu = 2 |\mu|^2.$$

Hence

$$\begin{aligned} \sigma(\bar{f})^2 &= \langle \bar{f}^* \bar{f} \rangle - \langle \bar{f} \rangle^* \langle \bar{f} \rangle \\ &= N^{-2} \left(N(\sigma^2 + |\mu|^2) + \binom{N}{2} 2 |\mu|^2 \right) - \mu^* \mu = N^{-1} \sigma^2, \end{aligned}$$

and the assertions follow. \square

5 Uncertainty

For you do not know which will succeed, whether this or that, or whether both will do equally well.

Kohelet, ca. 250 B.C. [44]

Due to our inability to prepare experiments with a sufficient degree of sharpness to know with certainty everything about a system we investigate, we need to describe the preparation of experiments in a stochastic language that permits the discussion of such uncertainties; in other words, we shall model prepared experiments by ensembles.

Formally, the essential difference between classical mechanics and quantum mechanics in the latter's lack of commutativity. While in classical mechanics there is in principle no lower limit to the uncertainties with which we can prepare the quantities in a system of interest, the quantum mechanical uncertainty relation for noncommuting quantities puts strict limits on the uncertainties in the preparation of microscopic ensembles. Here, *preparation* is defined informally as bringing the system into an ensemble such that measuring certain quantities gives values that agree with the expectation to an accuracy specified by given uncertainties.

In this section, we discuss the limits of the accuracy to which this can be done.

5.1 Proposition.

(i) **The Cauchy–Schwarz inequality**

$$|\langle f^* g \rangle|^2 \leq \langle f^* f \rangle \langle g^* g \rangle$$

holds for all $f, g \in \mathbb{E}$.

(ii) **The uncertainty relation**

$$\sigma(f)^2\sigma(g)^2 \geq |\text{cov}(f, g)|^2 + \left| \frac{1}{2}\langle f^*g - g^*f \rangle \right|^2$$

holds for all $f, g \in \mathbb{E}$.

(iii) For $f, g \in \mathbb{E}$,

$$\text{cov}(f, g) = \text{cov}(g, f) = \frac{1}{2}(\sigma(f+g)^2 - \sigma(f)^2 - \sigma(g)^2), \quad (16)$$

$$|\text{cov}(f, g)| \leq \sigma(f)\sigma(g), \quad (17)$$

$$\sigma(f+g) \leq \sigma(f) + \sigma(g). \quad (18)$$

In particular,

$$|\langle fg \rangle - \langle f \rangle \langle g \rangle| \leq \sigma(f)\sigma(g) \quad \text{for commuting Hermitian } f, g. \quad (19)$$

Proof. (i) For arbitrary $\alpha, \beta \in \mathbb{C}$ we have

$$\begin{aligned} 0 &\leq \langle (\alpha f - \beta g)^*(\alpha f - \beta g) \rangle \\ &= \alpha^* \alpha \langle f^* f \rangle - \alpha^* \beta \langle f^* g \rangle - \beta^* \alpha \langle g^* f \rangle + \beta^* \beta \langle g^* g \rangle \\ &= |\alpha|^2 \langle f^* f \rangle - 2 \text{Re}(\alpha^* \beta \langle f^* g \rangle) + |\beta|^2 \langle g^* g \rangle \end{aligned}$$

We now choose $\beta = \langle f^* g \rangle$, and obtain for arbitrary real α the inequality

$$0 \leq \alpha^2 \langle f^* f \rangle - 2\alpha |\langle f^* g \rangle|^2 + |\langle f^* g \rangle|^2 \langle g^* g \rangle. \quad (20)$$

The further choice $\alpha = \langle g^* g \rangle$ gives

$$0 \leq \langle g^* g \rangle^2 \langle f^* f \rangle - \langle g^* g \rangle |\langle f^* g \rangle|^2.$$

If $\langle g^* g \rangle > 0$, we find after division by $\langle g^* g \rangle$ that (i) holds. And if $\langle g^* g \rangle \leq 0$ then $\langle g^* g \rangle = 0$ and we have $\langle f^* g \rangle = 0$ since otherwise a tiny α produces a negative right hand side in (20). Thus (i) also holds in this case.

(ii) Since $(f - \bar{f})^*(g - \bar{g}) - (g - \bar{g})^*(f - \bar{f}) = f^*g - g^*f$, it is sufficient to prove the uncertainty relation for the case of quantities f, g whose expectation vanishes. In this case, (i) implies

$$(\text{Re}\langle f^*g \rangle)^2 + (\text{Im}\langle f^*g \rangle)^2 = |\langle f^*g \rangle|^2 \leq \langle f^*f \rangle \langle g^*g \rangle = \sigma(f)^2\sigma(g)^2.$$

The assertion follows since $\text{Re}\langle f^*g \rangle = \text{cov}(f, g)$ and

$$i \text{Im}\langle f^*g \rangle = \frac{1}{2}(\langle f^*g \rangle - \langle f^*g \rangle^*) = \frac{1}{2}\langle f^*g - g^*f \rangle.$$

(iii) Again, it is sufficient to consider the case of quantities f, g whose expectation vanishes. Then

$$\begin{aligned}\sigma(f+g)^2 &= \langle (f+g)^*(f+g) \rangle = \langle f^*f \rangle + \langle f^*g + g^*f \rangle + \langle g^*g \rangle \\ &= \sigma(f)^2 + 2\text{cov}(f, g) + \sigma(g)^2,\end{aligned}\tag{21}$$

and (16) follows. (17) is an immediate consequence of (ii), and (18) follows easily from (21) and (17). Finally, (19) is a consequence of (17) and Proposition 4.3(iii). \square

In the classical case of commuting Hermitian quantities, the uncertainty relation just reduces to the well-known inequality (17) of classical statistics. For noncommuting Hermitian quantities, the uncertainty relation is stronger. In particular, we may deduce from the commutation relation (11) for position q and momentum p HEISENBERG's [31, 67] uncertainty relation

$$\sigma(q)\sigma(p) \geq \frac{1}{2}\hbar.\tag{22}$$

Thus *no ensemble exists where both p and q have arbitrarily small standard deviation*. (More general noncommuting Hermitian quantities f, g may have *some* ensembles with $\sigma(f) = \sigma(g) = 0$, namely among those with $\langle fg \rangle = \langle gf \rangle$.)

Putting $k = \bar{p}$ and $x = \bar{q}$ and taking expectations in (13) and using Proposition 4.3(iii), we find another version of the uncertainty relation, implying again that $\sigma(p)$ and $\sigma(q)$ cannot be made simultaneously very small:

$$\left(\frac{\sigma(p)}{\Delta p}\right)^2 + \left(\frac{\sigma(q)}{\Delta q}\right)^2 \geq \frac{\hbar}{\Delta p \Delta q}.\tag{23}$$

Heisenberg's relation (22) follows from it by putting $\Delta p = \sigma(p)$ and $\Delta q = \sigma(q)$.

We now derive a characterization of the quantities f with vanishing uncertainty, $\sigma(f) = 0$; in classical probability theory these correspond to quantities (random variables) that have fixed values in every realization.

5.2 Definition. We say a quantity f **vanishes** in the ensemble $\langle \cdot \rangle$ if

$$\langle f^*f \rangle = 0.$$

5.3 Theorem.

- (i) $\sigma(f) = 0$ iff $f - \langle f \rangle$ vanishes.
- (ii) If f vanishes in the ensemble $\langle \cdot \rangle$ then $\langle f \rangle = 0$.

(iii) The set V of vanishing quantities satisfies

$$f + g \in V \quad \text{if } f, g \in V,$$

$$fg \in V \quad \text{if } g \in V \text{ and } f \in \mathbb{E} \text{ is bounded,}$$

$$f^2 \in V \quad \text{if } f \in V \text{ is Hermitian.}$$

Proof. (i) holds since $g = f - \langle f \rangle$ satisfies $\langle g^* g \rangle = \sigma(f)^2$.

(ii) follows from Proposition 4.3(ii).

(iii) If $f, g \in V$ then $\langle f^* g \rangle = 0$ and $\langle g^* f \rangle = 0$ by the Cauchy-Schwarz inequality, hence $\langle (f + g)^* (f + g) \rangle = \langle f^* f \rangle + \langle g^* g \rangle = 0$, so that $f + h \in V$.

If $g \in V$ and f is bounded then

$$(fg)^*(fg) = g^* f^* f g \leq g^* \|f\|^2 g = \|f\|^2 g^* g$$

implies $\langle (fg)^*(fg) \rangle \leq \|f\|^2 \langle g^* g \rangle = 0$, so that $fg \in V$.

And if $f \in V$ is Hermitian then $\langle f^2 \rangle = \langle f^* f \rangle = 0$, and, again by Cauchy-Schwarz, $\langle f^4 \rangle \leq \langle f^6 \rangle \langle f^2 \rangle = 0$, so that $f^2 \in V$. \square

6 Nonlocality

As the heavens are higher than the earth, so are my ways higher than your ways and my thoughts than your thoughts.

The LORD, according to Isaiah, ca. 540 B.C. [37]

Before they call I will answer; while they are still speaking I will hear.

The LORD, according to Isaiah, ca. 540 B.C. [38]

A famous feature of quantum physics is its intrinsic nonlocality, expressed by so-called **Bell inequalities** (cf. BELL [2], CLAUSER & SHIMONY [12]). The formulation given here depends on the most orthodox part of quantum mechanics only; it does not, as is usually done, refer to hidden variables, and involves no counterfactual reasoning.

6.1 Theorem. *Let f_k ($k = 1, 2, 3, 4$) be Hermitian quantities satisfying*

$$f_k^2 \leq 1 \quad \text{for } k = 1, 2, 3, 4. \tag{24}$$

(i) (cf. CIREL'SON [10]) For every ensemble,

$$|\langle f_1 f_2 \rangle + \langle f_3 f_2 \rangle + \langle f_3 f_4 \rangle - \langle f_1 f_4 \rangle| \leq 2\sqrt{2}. \quad (25)$$

(ii) (cf. CLAUSER et al. [11]) If, for odd $j - k$, the quantities f_j and f_k commute and are uncorrelated then

$$|\langle f_1 f_2 \rangle + \langle f_3 f_2 \rangle + \langle f_3 f_4 \rangle - \langle f_1 f_4 \rangle| \leq 2. \quad (26)$$

Proof. (i) Write γ for the left hand side of (25). Using the Cauchy-Schwarz inequality and the easily verified inequality

$$\sqrt{\alpha} + \sqrt{\beta} \leq \sqrt{2(\alpha + \beta)} \quad \text{for all } \alpha, \beta \geq 0,$$

we find

$$\begin{aligned} \gamma &= |\langle f_1(f_2 - f_4) \rangle + \langle f_3(f_2 + f_4) \rangle| \\ &\leq \sqrt{\langle f_1^2 \rangle \langle (f_2 - f_4)^2 \rangle} + \sqrt{\langle f_3^2 \rangle \langle (f_2 + f_4)^2 \rangle} \\ &\leq \sqrt{\langle (f_2 - f_4)^2 \rangle} + \sqrt{\langle (f_2 + f_4)^2 \rangle} \\ &\leq \sqrt{2(\langle (f_2 - f_4)^2 \rangle + \langle (f_2 + f_4)^2 \rangle)} = \sqrt{4\langle f_2^2 + f_4^2 \rangle} = \sqrt{8}. \end{aligned}$$

(ii) By Proposition 4.3(ii), $v_k := \langle f_k \rangle$ satisfies $|v_k| \leq 1$. If f_j and f_k commute and are uncorrelated for odd $j - k$ then Proposition 4.3(iv) implies $\langle f_j f_k \rangle = v_j v_k$ for odd $j - k$. Hence

$$\begin{aligned} \gamma &= |v_1 v_2 + v_3 v_2 + v_3 v_4 - v_1 v_4| = |v_1(v_2 - v_4) + v_3(v_2 + v_4)| \\ &\leq |v_1| |v_2 - v_4| + |v_3| |v_2 + v_4| \leq |v_2 - v_4| + |v_2 + v_4| \\ &= 2 \max(|v_2|, |v_4|) \leq 2. \end{aligned}$$

□

6.2 Example. In $\mathbb{C}^{4 \times 4}$, the four monomial matrices f_j defined by

$$f_1 x = \begin{pmatrix} x_3 \\ x_4 \\ x_1 \\ x_2 \end{pmatrix}, \quad f_2 x = \begin{pmatrix} x_2 \\ x_1 \\ x_4 \\ x_3 \end{pmatrix}, \quad f_3 x = \begin{pmatrix} x_1 \\ x_2 \\ -x_3 \\ -x_4 \end{pmatrix}, \quad f_4 x = \begin{pmatrix} x_1 \\ -x_2 \\ x_3 \\ -x_4 \end{pmatrix}$$

satisfy (24), and f_j and f_k commute and are uncorrelated for odd $j - k$. It is easily checked that in the pure ensemble defined by the vector

$$\psi = \begin{pmatrix} \alpha_1 \\ -\alpha_2 \\ \alpha_2 \\ \alpha_1 \end{pmatrix}, \quad \alpha_{1,2} = \sqrt{\frac{2 \pm \sqrt{2}}{8}},$$

$\langle f_1 f_2 \rangle = \langle f_3 f_2 \rangle = \langle f_3 f_4 \rangle = -\langle f_1 f_4 \rangle = \frac{1}{2}\sqrt{2}$. Hence (25) holds with equality and (26) is violated. Indeed, since $\langle f_k \rangle = 0$ for all k , we see that f_j and f_k are correlated for odd $j - k$.

On identifying

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \end{pmatrix}$$

and defining the tensor product action $u \otimes v : x \mapsto uxv^T$, the matrices f_j can be written in terms of the Pauli spin matrices (10) as

$$f_1 = \sigma_1 \otimes 1, \quad f_2 = 1 \otimes \sigma_1, \quad f_3 = \sigma_3 \otimes 1, \quad f_4 = 1 \otimes \sigma_3.$$

If we interpret the two terms in a tensor product as quantities related to two spatially separated fermion particles A and B , we conclude that there are pure ensembles in which the components of the spin vectors of two fermion particles are correlated, no matter how far apart the two particles are placed.

Such *nonlocal correlations* of certain quantum ensembles are an enigma of the microscopic world that, being experimentally confirmed, cannot be removed by any interpretation of quantum mechanics. (See BELL [2] for the original Bell inequality, PITOWSKY [63] for a treatise on Bell inequalities, and ASPECT [1], CLAUSER & SHIMONY [12], TITTEL et al. [74] for experiments verifying the violation of (26).)

7 Probability

Enough, if we adduce probabilities as likely as any others; for we must remember that I who am the speaker, and you who are the judges, are only mortal men, and we ought to accept the tale which is probable and enquire no further.
Plato, ca. 367 B.C. [64]

The interpretation of probability has been surrounded by philosophical puzzles for a long time. FINE [23] is probably still the best discussion of the problems involved; HACKING [27] gives a good account of its early history. (See also HOME AND WHITAKER [36].) Our definition generalizes the classical intuition of probabilities as weights in a weighted average and is modeled after the formula for finite probability theory in Example 4.2(i).

In the special case when a well-defined counting process may be associated with the statement whose probability is assessed, our exposition supports the conclusion of DRIESCHNER [16, p.73], “*probability is predicted relative frequency*” (German original: “Wahrscheinlichkeit ist vorausgesagte relative Häufigkeit”). More specifically, we assert that, *for counting events, the probability carries the information of expected relative frequency* (see Theorem 7.4(iii) below).

To make this precise we need a precise concept of independent events that may be counted. To motivate our definition, assume that we look at times t_1, \dots, t_N for the presence of an event of the sort we want to count. We introduce quantities e_l whose value is the amount added to the counter at time t_l . For correct counting, we need $e_l \approx 1$ if an event happened at time t_l , and $e_l \approx 0$ otherwise; thus e_l should have the two possible values 0 and 1 only. Since these numbers are precisely the Hermitian idempotents among the constant quantities, this suggests to identify events with general Hermitian idempotent quantities.

In addition, it will be useful to have the more general concept of ‘effects’ for more fuzzy, event-like things.

7.1 Definition.

(i) A quantity $e \in \mathbb{E}$ satisfying $0 \leq e \leq 1$ is called an **effect**. The number $\langle e \rangle$ is called the **probability** of the effect e . Two effects e, e' are called **independent** in an ensemble $\langle \cdot \rangle$ if they commute and satisfy

$$\langle ee' \rangle = \langle e \rangle \langle e' \rangle.$$

(ii) A quantity $e \in \mathbb{E}$ satisfying $e^2 = e = e^*$ is called an **event**. Two events e, e' are called **disjoint** if $ee' = e'e = 0$.

(iii) An **alternative** is a family e_l ($l \in L$) of effects such that

$$\sum_{l \in L} e_l \leq 1.$$

7.2 Proposition.

- (i) Every event is an effect.
- (ii) The probability of an effect e satisfies $0 \leq \langle e \rangle \leq 1$.
- (iii) The set of all effects is convex and closed in the uniform topology.
- (iv) Any two events in an alternative are disjoint.

Proof. (i) holds since $0 \leq e^*e = e^2 = e$ and $0 \leq (1-e)^*(1-e) = 1 - 2e + e^2 = 1 - e$.

(ii) and (iii) follow easily from Proposition 4.3.

(iv) If e_k, e_l are events in an alternative then $e_k \leq 1 - e_l$ and

$$(e_k e_l)^*(e_k e_l) = e_l^* e_k^* e_k e_l = e_l^* e_k^2 e_l = e_l^* e_k e_l \leq e_l^* (1 - e_l) e_l = 0.$$

Hence $e_k e_l = 0$ and $e_l e_k = e_l^* e_k^* = (e_k e_l)^* = 0$. \square

Note that we have a well-defined notion of probability though the concept of a probability distribution is absent. It is neither needed nor definable in general. Nevertheless, the theory contains classical probability theory as a special case.

7.3 Examples.

(i) **Classical probability theory.** In classical probability theory, quantities are usually called **random variables**; they belong to the Q-algebra $B(\Omega)$ of measurable complex-valued functions on a measurable set Ω .

The characteristic function $e = \chi_M$ of any measurable subset M of Ω (with $\chi_M(\omega) = 1$ if $\omega \in M$, $\chi_M(\omega) = 0$ otherwise) is an event. A family of characteristic functions χ_{M_l} form an alternative iff their supports M_l are pairwise disjoint.

Effects are the measurable functions e with values in $[0, 1]$; they can be considered as ‘characteristic functions’ of a fuzzy set where $\omega \in \Omega$ has $e(\omega)$ as degree of membership (see, e.g., ZIMMERMANN [80]).

For many applications, the algebra $B(\Omega)$ is too big, and suitable subalgebras \mathbb{E} are selected on which the relevant ensembles can be defined as integrals with respect to suitable positive measures.

(ii) **Quantum probability theory.** In the algebra of bounded linear operators on a Hilbert space \mathbb{H} , every unit vector $\varphi \in \mathbb{H}$ gives rise to an **elementary event** $e_\varphi = \varphi\varphi^*$. A family of elementary events e_{φ_l} form an alternative iff the φ_l are pairwise orthogonal. The probability of an elementary event e_φ in an ensemble corresponding to the unit vector ψ is

$$\langle e_\varphi \rangle = \psi^* e_\varphi \psi = \psi^* \varphi \varphi^* \psi = |\varphi^* \psi|^2. \quad (27)$$

This is the well-known **squared probability amplitude** formula, traditionally interpreted as the probability that after preparing a pure ensemble in ‘state’ ψ , an ideal measurement causes a ‘state reduction’ to the new pure ‘state’ φ . Note that our interpretation of $|\varphi^* \psi|^2$ is completely within the formal framework of the theory and completely independent of the measurement process.

Further, nonelementary quantum events are orthogonal projectors to subspaces. The effects are the Hermitian operators e with spectrum in $[0, 1]$.

7.4 Theorem.

(i) For any effect e , its **negation** $\neg e = 1 - e$ is an effect with probability

$$\langle \neg e \rangle = 1 - \langle e \rangle;$$

it is an event if e is an event.

(ii) For commuting effects e, e' , the quantities

$$e \wedge e' = ee' \quad (e \text{ and } e'),$$

$$e \vee e' = e + e' - ee' \quad (e \text{ or } e')$$

are effects whose probabilities satisfy

$$\langle e \wedge e' \rangle + \langle e \vee e' \rangle = \langle e \rangle + \langle e' \rangle;$$

they are events if e, e' are events. Moreover,

$$\langle e \wedge e' \rangle = \langle e \rangle \langle e' \rangle \quad \text{for independent effects } e, e'.$$

(iii) For a family of effects e_l ($l = 1, \dots, N$) with constant probability $\langle e_l \rangle = p$, the **relative frequency**

$$q := \frac{1}{N} \sum_{l=1}^N e_l$$

satisfies

$$\langle q \rangle = p.$$

(iv) For a family of independent events of probability p , the uncertainty

$$\sigma(q) = \sqrt{\frac{p(1-p)}{N}}$$

of the relative frequency becomes arbitrarily small as N becomes sufficiently large (**weak law of large numbers**).

Proof. (i) $\neg e$ is an effect since $0 \leq 1 - e \leq 1$, and its probability is $\langle \neg e \rangle = \langle 1 - e \rangle = 1 - \langle e \rangle$. If e is an event then clearly $\neg e$ is Hermitian, and $(\neg e)^2 = (1 - e)^2 = 1 - 2e + e^2 = 1 - e = \neg e$. Hence $\neg e$ is an event.

(ii) Since e and e' commute, $e \wedge e' = ee' = e^2 e' = ee' e$. Since $ee' e \geq 0$ and $ee' e \leq ee = e \leq 1$, we see that $e \wedge e'$ is an effect. Therefore, $e \vee e' = e + e' - ee' =$

$1 - (1 - e)(1 - e') = \neg(\neg e \wedge \neg e')$ is also an effect. The assertions about expectations are immediate. If e, e' are events then $(ee')^* = e'^*e^* = e'e = ee'$, hence ee' is Hermitian; and it is idempotent since $(ee')^2 = ee'ee' = e^2e'^2 = ee'$. Therefore $e \wedge e' = ee'$ is an event, and $e \vee e' = \neg(\neg e \wedge \neg e')$ is an event, too.

(iii) This is immediate by taking the expectation of q .

(iv) This follows from Theorem 4.4 since $\langle e_k^2 \rangle = \langle e_k \rangle = p$ and

$$\sigma(e_k)^2 = \langle (e_k - p)^2 \rangle = \langle e_k^2 \rangle - 2p\langle e_k \rangle + p^2 = p - 2p^2 + p^2 = p(1 - p).$$

□

We remark in passing that, with the operations \wedge, \vee, \neg , the set of events in any *commutative* subalgebra of \mathbb{E} forms a Boolean algebra; see STONE [71]. Traditional quantum logic (see, e.g., BIRKHOFF & VON NEUMANN [5], PITOWSKY [63], SVOZIL [73]) discusses the extent to which this can be generalized to the noncommutative case. We shall make no use of quantum logic; the only logic used is classical logic, applied to well-defined assertions about quantities. However, certain facets of quantum logic related to so-called ‘hidden variables’ are discussed from a different point of view in the next section.

The set of effects in a commutative subalgebra is *not* a Boolean algebra. Indeed, $e \wedge e \neq e$ for effects e that are not events. In fuzzy set terms, if e codes the answer to the question ‘(to which degree) is statement S true?’ then $e \wedge e$ codes the answer to the question ‘(to which degree) is statement S really true?’, indicating the application of more stringent criteria for truth.

For noncommuting effects, ‘and’ and ‘or’ are undefined. One might think of $\frac{1}{2}(ee' + e'e)$ as a natural definition for $e \wedge e'$; however, this expression need not be an event, as the simple example

$$e = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad e' = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \frac{1}{2}(ee' + e'e) = \frac{1}{4} \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}$$

shows.

8 States

For example, nobody doubts that at any given time the center of mass of the Moon has a definite position, even in the absence of any real or potential observer.

Albert Einstein [19]

States formalize the objective properties that physical systems possess. We consider properties (the ‘beables’ of BELL [3]) to be assignments of complex numbers $v(f)$ to certain quantities f .

The specification of which states correspond to physical systems is part of the interpretation problem of quantum mechanics. Different schools use different proposals but, due to the lack of experimental tests, no agreement has been reached. We therefore demand only minimal requirements shared by all reasonable concepts of states, and independent on any a priori relations to (as yet undefined) measurement.

We discuss the constraints imposed on sharpness, a desirable property of Hermitian quantities. In this way we find an answer to the question: Assuming there is an objective reality behind quantum physics, what form can it take?

Since not all states assign properties to all quantities, we need a symbol ‘?’ that indicates an unspecified (and perhaps undefined) value. Operations involving ? give ? as a result, with exception of the rule

$$0? = ?0 = 0.$$

8.1 Definition.

(i) A **state** is a mapping $v : \mathbb{E} \rightarrow \mathbb{C} \cup \{?\}$ such that

$$(S1) \quad v(\alpha + \beta f) = \alpha + \beta v(f) \quad \text{if } \alpha, \beta \in \mathbb{C},$$

$$(S2) \quad v(f) \in \mathbb{R} \cup \{?\} \quad \text{if } f \text{ is Hermitian.}$$

$v(f)$ is called the **reference value** of f in state v . $\mathbb{E}_v := \{f \in \mathbb{E} \mid v(f) \in \mathbb{C}\}$ denotes the set of quantities with definite values in state v .

(ii) A set E of Hermitian quantities is called **sharp** in state v if, for $f, g \in E$ and $\lambda \in \mathbb{R}$,

$$(SQ0) \quad \mathbb{R} \subseteq E, \quad v(f) \in \mathbb{R},$$

$$(SQ1) \quad f^2 \in E, \quad v(f^2) = v(f)^2,$$

$$(SQ2) \quad f^{-1} \in E, \quad v(f^{-1}) = v(f)^{-1} \quad \text{if } f \text{ is invertible,}$$

$$(SQ3) \quad f \pm g \in E, \quad v(f + \lambda g) = v(f) + \lambda v(g) \quad \text{if } f, g \text{ commute.}$$

A quantity f is called **sharp** in v if $\text{Re } f$ and $\text{Im } f$ commute and belong to some set that is sharp in state v .

Thus, sharp quantities behave with respect to their reference values precisely as numbers would do. In particular, sharp quantities are normal by Corollary 2.4.

While having a well-defined reference value guarantees objectivity and hence observer-independent reality, sharpness is a matter not of objectivity but one of point-like behavior.

8.2 Examples.

(i) **Classical mechanics.** Classical N -particle mechanics is described by a *phase space* Ω_{cl} , the direct product of $\mathbb{R}^N \times \mathbb{R}^N$ and a compact manifold describing internal particle degrees of freedom. \mathbb{E} is a subalgebra of the algebra $B(\Omega_{cl})$ of Borel measurable functions on **phase space** Ω_{cl} .

A **classical point state** is defined for each $\omega \in \Omega_{cl}$ by

$$v_\omega(f) := \begin{cases} f(\omega) & \text{if } f \text{ is continuous at } \omega, \\ ? & \text{otherwise.} \end{cases}$$

In a classical point state v , all $f \in \mathbb{E}_v$ are sharp (and normal).

(ii) **Nonrelativistic quantum mechanics.** Nonrelativistic quantum mechanics of N particles is described by a Hilbert space $\mathbb{H} = L^2(\Omega_{qu})$, where Ω_{qu} is the direct product of \mathbb{R}^N and a finite set that takes care of spin, color, and similar indices. $\mathbb{E} = \mathbb{E}_2(\Omega)$ is the algebra of bounded linear operators on \mathbb{H} . (If unbounded operators are considered, \mathbb{E} is instead an algebra of linear operators in the corresponding Schwartz space, but for this example, we don't want to go into technical details.)

The Copenhagen interpretation is the most prominent, and at the same time the most restrictive interpretation of quantum mechanics. It assigns definite values only to quantities in an eigenstate. A **Copenhagen state** is defined for each $\psi \in \mathbb{H} \setminus \{0\}$ by

$$v_\psi(f) := \begin{cases} \lambda & \text{if } f\psi = \lambda\psi, \\ ? & \text{otherwise.} \end{cases}$$

In a Copenhagen state v , all normal $f \in \mathbb{E}_v$ are sharp.

Our first observation is that numbers are their own reference values, and that sharp events are dichotomic – their only possible reference values are 0 and 1.

8.3 Proposition.

- (i) $v(\alpha) = \alpha$ if $\alpha \in \mathbb{C}$.
- (ii) If e is a sharp event then $v(e) \in \{0, 1\}$.

Proof. (i) is the case $\beta = 0$ of (S1), and (ii) holds since in this case, (SQ1) implies $v(e) = v(e^2) = v(e)^2$. \square

8.4 Proposition. If the set E is sharp in the state v then

$$fg \in E, \quad v(fg) = v(f)v(g) \quad \text{if } f, g \in E \text{ commute,} \quad (28)$$

$$\alpha + \beta f \in E, \quad v(\alpha + \beta f) = \alpha + \beta v(f) \quad \text{if } f \in E, \alpha, \beta \in \mathbb{R}. \quad (29)$$

Proof. If $f, g \in E$ commute then $f \pm g \in E$ by (SQ3). By (SQ1), $(f \pm g)^2 \in E$ and $v((f \pm g)^2) = v(f \pm g)^2$. By (SQ3), $fg = ((f + g)^2 - (f - g)^2)/4$ belongs to E and satisfies

$$\begin{aligned} 4v(fg) &= v((f + g)^2) - v((f - g)^2) = v(f + g)^2 - v(f - g)^2 \\ &= (v(f) + v(g))^2 - (v(f) - v(g))^2 = 4v(f)v(g). \end{aligned}$$

Thus (28) holds, and (29) follows from (28), (SQ0) and (SQ3). \square

One of the nontrivial traditional *postulates* of quantum mechanics, that the possible values a sharp quantity f may take are the elements of the spectrum $\text{Spec } f$ of f , is a *consequence* of our axioms.

8.5 Theorem. If a Hermitian quantity f is sharp with respect to v , and $v(f) = \lambda$ then:

- (i) $\lambda - f$ is not invertible.
- (ii) If there is a polynomial $\pi(x)$ such that $\pi(f) = 0$ then λ satisfies $\pi(\lambda) = 0$. In particular, if f is a sharp event then $v(f) \in \{0, 1\}$.
- (iii) If \mathbb{E} is finite-dimensional then there is a quantity $g \neq 0$ such that $fg = \lambda g$, i.e., λ is an eigenvalue of f .

Proof. Note that λ is real by (SQ0).

- (i) If $g := (\lambda - f)^{-1}$ exists then by (29) and (SQ2), $\lambda - f, g \in E$ and

$$v(\lambda - f)v(g) = v((\lambda - f)g) = v(1) = 1,$$

contradicting $v(\lambda - f) = \lambda - v(f) = 0$.

(ii) By polynomial division we can find a polynomial $\pi_1(x)$ such that $\pi(x) = \pi(\lambda) + (x - \lambda)\pi_1(x)$. If $\pi(\lambda) \neq 0$, $g := -\pi_1(f)/\pi(\lambda)$ satisfies

$$(\lambda - f)g = (f - \lambda)\pi_1(f)/\pi(\lambda) = (\pi(\lambda) - \pi(f))/\pi(\lambda) = 1,$$

hence $\lambda - f$ is invertible with inverse g , contradiction. Hence $\pi(\lambda) = 0$. In particular, this applies to an event with $\pi(x) = x^2 - x$; hence its possible reference values are zeros of $\pi(x)$, i.e., either 0 or 1.

(iii) The powers f^k ($k = 0, \dots, \dim \mathbb{E}$) must be linearly dependent; hence there is a polynomial $\pi(x)$ such that $\pi(f) = 0$. If this is chosen of minimal degree then $g := \pi_1(f)$ is nonzero since its degree is too small. Since $0 = \pi(\lambda) = \pi(f) + (f - \lambda)\pi_1(f) = (f - \lambda)g$, we have $fg = \lambda g$. \square

When \mathbb{E} is a C^* -algebra, the spectrum of $f \in \mathbb{E}$ is defined as the set of complex numbers λ such that $\lambda - f$ has no inverse (see, e.g., [66]). Thus in this case, part (i) of the theorem implies that all numerical values a sharp quantity f can take belong to the spectrum of f . This covers both the case of classical mechanics and that of nonrelativistic quantum mechanics.

However, in general, one cannot hope that *every* Hermitian quantity is sharp. Indeed, it was shown already by KOCHEN & SPECKER [42] that there is a finite set of events in $\mathbb{C}^{3 \times 3}$ (and hence in $\mathbb{C}^{n \times n}$ for all $n \geq 3$) for which any assignment of reference values leads to a contradiction with the sharpness conditions. We give a slightly less general result that is much easier to prove.

8.6 Theorem. (cf. MERMIN [47], PERES [61])

There is no state with a sharp set of quantities containing four Hermitian quantities f_j ($j = 1, 2, 3, 4$) satisfying $f_j^2 = 1$ and

$$f_j f_k = \begin{cases} -f_k f_j & \text{if } j - k = \pm 2, \\ f_k f_j & \text{otherwise.} \end{cases} \quad (30)$$

Proof. Let E be a set containing the f_j . If E is sharp in the state v then $v_j = v(f_j)$ is a number, and $v_j^2 = v(f_j^2) = v(1) = 1$ implies $v_j \in \{-1, 1\}$. In particular, $v_0 := v_1 v_2 v_3 v_4 \in \{-1, 1\}$. By (28), $v(f_j f_k) = v_j v_k$ if $j, k \neq \pm 2$. Since $f_1 f_2$ and $f_3 f_4$ commute, $v(f_1 f_2 f_3 f_4) = v(f_1 f_2) v(f_3 f_4) = v_1 v_2 v_3 v_4 = v_0$, and since $f_1 f_4$ and $f_2 f_3$ commute, $v(f_1 f_4 f_2 f_3) = v(f_1 f_4) v(f_2 f_3) v_1 v_4 v_2 v_3 = v_0$. Since $f_1 f_4 f_2 f_3 = -f_1 f_2 f_3 f_4$, this gives $v_0 = -v_0$, hence the contradiction $v_0 = 0$. \square

8.7 Example. The 4×4 -matrices f_j defined in Example 6.2 satisfy the required relations. In particular, there cannot be a state in which all components of the spin vectors of two fermions are sharp.

This is the basic reason underlying a number of well-known arguments against so-called local hidden variable theories, which assume that *all* Hermitian quantities are sharp. (See BERNSTEIN [4], EBERHARD [17], GREENBERGER et al. [25, 26], HARDY [28, 29], MERMIN [47, 48], PERES [60, 61], VAIDMAN [75]). For a treatment in terms of quantum logic, see SVOZIL [73].

Sharp quantities always satisfy a **Bell inequality** analogous to inequality (26) for uncorrelated quantities:

8.8 Theorem. *Let v be a state with a sharp set of quantities containing four Hermitian quantities f_j ($j = 1, 2, 3, 4$) satisfying $f_j^2 = 1$ and $[f_j, f_k] = 0$ for odd $j - k$. Then*

$$|v(f_1 f_2) + v(f_2 f_3) + v(f_3 f_4) - v(f_1 f_4)| \leq 2. \quad (31)$$

Proof. Let $v_k := v(f_k)$. Then (SQ2) implies $v_k^2 = v(f_k^2) = v(1) = 1$, and since equation (28) implies $v(f_j f_k) = v_j v_k$ for odd $j - k$, we find

$$\begin{aligned} \gamma &= |v_1 v_2 + v_2 v_3 + v_3 v_4 - v_1 v_4| \\ &= |v_1(v_2 - v_4) + v_3(v_2 + v_4)| \\ &\leq |v_1| |v_2 - v_4| + |v_3| |v_2 + v_4| \\ &\leq |v_2 - v_4| + |v_2 + v_4| \\ &= 2 \max(|v_2| + |v_4|) \leq 2. \end{aligned}$$

□

Note, however, that Example 8.7 already implies that the sharpness assumption in this theorem (and in other derivations of Bell inequalities for local hidden variable theories; see, e.g., the treatise PITOWSKY [63]) fails not only in special entangled ensembles such as that exhibited in Example 6.2 but must fail independent of any special preparation.

While the above results show that one cannot hope to find quantum states in which all Hermitian quantities are sharp, results of CLIFTON & KENT [13] imply that one can achieve sharpness in $\mathbb{E} = \mathbb{C}^{n \times n}$ at least for a dense subset of Hermitian quantities.

9 States without squaring rule

*But if we have food and clothing, we will
be content with that.*

St. Paul, ca. 60 A.D. [59]

Since sharpness cannot be achieved for all Hermitian quantities, we discuss the relevance of the sharpness assumption.

The chief culprit among the sharpness assumptions seems to be the squaring rule (SQ1) from which the product rule (28) was derived. Indeed, the squaring rule (and hence the product rule) already fails in a simpler, classical situation, namely when considering weak limits of highly oscillating functions. For example, consider the family of functions f_k defined on $[0, 1]$ by $f_k(x) = \alpha$ if $\lfloor kx \rfloor$ is even and $f_k(x) = \beta$ if $\lfloor kx \rfloor$ is odd. Trivial integration shows that the weak-* limits are $\lim f_k = \frac{1}{2}(\alpha + \beta)$ and $\lim f_k^2 = \frac{1}{2}(\alpha^2 + \beta^2)$, and these do not satisfy the expected relation $\lim f_k^2 = (\lim f_k)^2$. Such weak limits of highly oscillating functions lead to the concept of a *Young measure*, which is of relevance in the calculus of variation of nonconvex functionals and in the physics of metal microstructure. See, e.g., ROUBICEK [68].

More insight from the classical regime comes from realizing that reference values are a microscopic analogue of similar macroscopic constructions.

For example, the center of mass, the mass-weighted average of the positions of the constituent particles, serves in classical mechanics as a convenient reference position of an extended object. It defines a point in space with a precise and objective physical meaning. The object is near this reference position, within an uncertainty given by the diameter of the object. Similarly, a macroscopic object has a well defined reference velocity, the mass-weighted average of the velocities of the constituent particles.

Thus, if we define an algebra \mathbb{E} of ‘intensive’ macroscopic mechanical quantities, given by all (mass-independent and sufficiently nice) functions of time t , position $q(t)$, velocity $\dot{q}(t)$ and acceleration $\ddot{q}(t)$, the natural reference value $v_{mac}(f)$ for a quantity f is the mass-weighted average of the f -values of the constituent particles (labeled by superscripts a),

$$v_{mac}(f) = \sum_a m^a f(t, q^a(t), \dot{q}^a(t), \ddot{q}^a(t)) / \sum_a m^a.$$

This reference value behaves correctly under aggregation, if on the right hand side the reference values of the aggregates are substituted, so that it is independent of the details of how the object is split into constituents. Moreover, $v = v_{mac}$ has nice properties: **unrestricted additivity**,

(SL) $v(f + g) = v(f) + v(g)$ if $f, g \in \mathbb{E}$,

and **monotony**,

(SM) $f \geq g \Rightarrow v(f) \geq v(g)$.

However, neither position nor velocity nor acceleration is a sharp quantity with respect to v_{mac} since (SQ1) and (SQ2) fail. Note that deviations from the squaring rule make physical sense; for example, $v_{mac}(\dot{q}^2) - v_{mac}(\dot{q})^2$ is (in thermodynamic equilibrium) proportional to the temperature of the system.

From this perspective, and in view of Einstein's quote at the beginning of section 8, demanding the squaring rule for a reference value is unwarranted since it does not even hold in this classical situation.

Once the squaring rule (and hence sharpness) is renounced as a requirement for definite reference values, the arena is free for interpretations that use reference values defined for *all* quantities, and thus give a satisfying realistic picture of quantum mechanics. In place of the lost multiplicative properties we may now require unrestricted additivity (SL) without losing interesting examples.

For example, the 'local expectation values' of Bohmian mechanics (BOHM [6]) have this property, if the prescription given for Hermitian quantities in HOLLAND [35, (3.5.4)] is extended to general quantities, using the formula

$$v(f) := v(\operatorname{Re} f) + iv(\operatorname{Im} f)$$

which follows from (SL). Such **Bohmian states** have, by design, sharp positions at all times. However, they lack desirable properties such as monotony (SM), and they display other counterintuitive behavior (see, e.g., NEUMAIER [52] and its references).

A much more natural proposal is to *require that each state is an ensemble*. Then (SL) and (SM) hold, and one even has a replacement for the multiplicative properties. Indeed, for such **ensemble states**, it follows from (19) that there is an uncertainty measure

$$\Delta f = \sqrt{v(f^2) - v(f)^2} \tag{32}$$

associated with each Hermitian quantity f such that

$$|v(fg) - v(f)v(g)| \leq \Delta f \Delta g \quad \text{for commuting Hermitian } f, g. \tag{33}$$

Thus the product rule (and in particular the squaring rule) holds in an approximate form.

For quantities with small uncertainty Δf , we have essentially classical (nearly sharp) behavior. In particular, by the weak law of large numbers, Theorem 4.4, averages over many uncorrelated commuting quantities of the same kind have small uncertainty and hence are nearly classical. In particular, this holds for the quantities considered in statistical mechanics, and *explains the emergence of classical properties for macroscopic systems*.

Indeed, in statistical mechanics, classical values for observables are traditionally defined as expectations, and the concept of ensemble states with objective reference values for all quantities simply extends this downwards to the quantum domain.

With the interpretation that the only states realized in quantum mechanics are ensemble states, *quantum objects are inherently extended objects*, and realizing this reduces the riddles the interpretation of the microworld poses when instead pointlike (sharp) properties are imagined.

9.1 Examples.

(i) **The ground state of hydrogen.** The uncertainty Δq of position (defined by interpreting (32) for the vector q in place of the scalar f) in the ground state of hydrogen is $\Delta q = \sqrt{3}r_0$ (where $r_0 = 5.29 \cdot 10^{-11}$ m is the Bohr radius of a hydrogen atom), slightly larger than the reference radius $v(r) = v(|q - v(q)|) = 1.5r_0$.

(ii) **The center of mass of the Moon.** The Moon has a mass of $m_{\text{Moon}} = 7.35 \cdot 10^{22}$ kg. Assuming the Moon consists mainly of silicates, we may take the average mass of an atom to be about 20 times the proton mass $m_p = 1.67 \cdot 10^{-27}$ kg. Thus the Moon contains about $N = m_{\text{Moon}}/20m_p = 2.20 \cdot 10^{48}$ atoms. In the rest frame of an observer standing on the Moon, the objective uncertainty of an atom position (due to the thermal motion of the atoms in the Moon) may be taken to be a small multiple of the Bohr radius r_0 . Assuming that the deviations from the reference positions are uncorrelated, we may use (15) to find as uncertainty of the position of the center of mass of the Moon a small multiple of $r_0/\sqrt{N} = 3.567 \cdot 10^{-35}$ m. Thus the center of mass of the Moon has a definite objective position, sharp within the measuring accuracy of many generations to come.

Ensemble states provide an elegant solution to the reality problem, confirming the insistence of the orthodox Copenhagen interpretation on that there is nothing but ensembles, while avoiding their elusive reality picture. It also conforms to OCKHAM's razor [56, 34], *frustra fit per plura quod potest fieri per pauciora*, that we should not use more degrees of freedom than are necessary to explain a phenomenon.

Quantum reality with reference values defined by ensemble states is as well-behaved and objective as classical macroscopic reality with reference values defined by a mass-weighted average over constituent values, and lacks sharpness (in the sense of our definition) to the same extent as classical macroscopic reality.

Moreover, classical point states are ensemble states, and whenever a Copenhagen state assigns a numerical value to a quantity, the corresponding pure ensemble state assigns the same value to it. Thus both classical mechanics and the orthodox interpretation of quantum mechanics are naturally embedded in the ensemble state interpretation.

The logical riddles of quantum mechanics (see, e.g., SVOZIL [73]) find their explanation in the fact that most events are unsharp in a given ensemble state, so that their objective reference values are no longer dichotomic but may take arbitrary values in $[0, 1]$, by (SM).

The arithmetical riddles of quantum mechanics (see, e.g., SCHRÖDINGER [69]) find their explanation in the fact that most Hermitian quantities are unsharp in a given ensemble state, so that their objective reference values are no longer eigenvalues but may take arbitrary values in the convex hull of the eigenvalues.

The geometric riddles of quantum mechanics – e.g., in the double slit experiment (BOHR [7], WOOTTERS & ZUREK [79]) and in EPR-experiments (ASPECT [1], CLAUSER & SHIMONY [12]) – do not disappear. But they remain within the magnitudes predicted by reference radii and uncertainties, hence require no special interpretation in the microscopic case. They simply demonstrate that particles are intrinsically extended and that electrons cannot be regarded as pointlike. (For photons, this is known to be the case also for different reasons, namely the nonexistence of a position operator with commuting components; see, e.g., STRNAD [72], MANDEL & WOLF [46, Chapter 12.11], NEWTON & WIGNER [55], PRYCE [65], but cf. HAWTON [30].)

Moreover, when considering quantum mechanical phenomena that violate our geometric intuition, one should bear in mind two similar violations of a naive geometric picture for the center of mass, Einstein’s prototype example for a definite and objective property of macroscopic systems:

First, though it is objective, the center of mass is nevertheless a fictitious point, not visibly distinguished in reality; for nonconvex objects it may even lie outside the object! Second, the center of mass follows a well-defined, objective path, though this path need not conform to the visual path of the object; this can be seen by pushing a long, elastic cylinder through a strongly

bent tube.

All these considerations are independent of the measurement problem. To investigate how measurements of classical macroscopic quantities (i.e., expectations of quantities with small uncertainty related to a measuring device) correlate with reference values of a microscopic system interacting with the device requires a precise definition of a measuring device and of the behavior of the combined system under the interaction (cf. the treatments in BUSCH et al. [8, 9], GIULINI et al. [24], MITTELSTAEDT [50] and PERES [62]). We shall discuss this problem from our perspective in a later part of this sequence of papers.

10 Dynamics

The lot is cast into the lap; but its every decision is from the LORD.

King Solomon, ca. 1000 B.C. [70]

God does not play dice with the universe.

Albert Einstein, 1927 A.D. [18]

In this section we discuss the most elementary aspects of the dynamics of (closed and isolated) physical systems. We shall have much more to say about dynamics in later parts of this series of papers, where so-called Poisson algebras will be used to make the formal dynamical parallels between classical mechanics and quantum mechanics understandable as two special cases of a single theory.

The observations about a physical system change with time. The dynamics of a closed and isolated physical system is conservative, and may be described by a fixed (but system-dependent) one-parameter family S_t ($t \in \mathbb{R}$) of **automorphisms** of the $*$ -algebra \mathbb{E} , i.e., mappings $S_t : \mathbb{E} \rightarrow \mathbb{E}$ satisfying (for $f, g \in \mathbb{E}$, $\alpha \in \mathbb{C}$, $s, t \in \mathbb{R}$)

$$(A1) \quad S_t(\alpha) = \alpha, \quad S_t(f^*) = S_t(f)^*,$$

$$(A2) \quad S_t(f + g) = S_t(f) + S_t(g), \quad S_t(fg) = S_t(f)S_t(g),$$

$$(A3) \quad S_0(f) = f, \quad S_{s+t}(f) = S_s(S_t(f)).$$

In the **Heisenberg picture** of the dynamics, where states are fixed and quantities change with time, $f(t) := S_t(f)$ denotes the time-dependent **Heisenberg quantity** associated with f at time t . Note that $f(t)$ is uniquely determined by $f(0) = f$. Thus the dynamics is deterministic, *independent of*

whether we are in a classical or in a quantum setting.

(In contrast, nonisolated closed systems are dissipative and intrinsically stochastic; see, e.g., GIULINI et al. [24]. We shall discuss this in a later part of this series.)

10.1 Examples. In nonrelativistic mechanics, conservative systems are described by a Hermitian quantity H , called the **Hamiltonian**.

(i) In **classical mechanics** – cf. Example 8.2(i) –, a Poisson bracket $\{\cdot, \cdot\}$ together with H defines the Liouville superoperator $Lf = \{f, H\}$, and the dynamics is given by the one-parameter group defined by

$$S_t(f) = e^{tL}(f),$$

corresponding to the differential equation

$$\frac{df(t)}{dt} = \{f(t), H\}. \quad (34)$$

(ii) In **nonrelativistic quantum mechanics** – cf. Example 8.2(ii) –, the dynamics is given by the one-parameter group defined by

$$S_t(f) = e^{-tH/i\hbar} f e^{tH/i\hbar},$$

corresponding to the **Heisenberg equation**

$$i\hbar \frac{df(t)}{dt} = e^{-tH/i\hbar} [f, H] e^{tH/i\hbar} = [f(t), H]. \quad (35)$$

(iii) **Relativistic quantum mechanics** is currently (for interacting systems) developed only for scattering events in which the dynamics is restricted to transforming quantities of a system at $t = -\infty$ to those at $t = +\infty$ by means of a single automorphism S given by

$$S(f) = s f s^*,$$

where s is a unitary quantity (i.e., $ss^* = s^*s = 1$), the so-called **scattering matrix**, for which an asymptotic series in powers of \hbar is computable from quantum field theory.

The realization of the axioms is different in the classical and in the quantum case, but the interpretation is identical.

The common form and deterministic nature of the dynamics, independent of any assumption of whether the system is classical or quantum, implies

that there is no difference in the causality of classical mechanics and that of quantum mechanics. Therefore, *the differences between classical mechanics and quantum mechanics cannot lie in an assumed intrinsic indeterminacy of quantum mechanics contrasted to deterministic classical mechanics.* The only difference between classical mechanics and quantum mechanics in the latter's lack of commutativity.

Of course, reference values of quantities at different times will generally be different. To see what happens, suppose that, in state v , a quantity f has reference value $v(f)$ at time $t = 0$. At time t , the quantity f developed into $f(t)$, with reference value

$$v(f(t)) = v(S_t(f)) = v_t(f), \quad (36)$$

where the time-dependent **Schrödinger state**

$$v_t = v \circ S_t \quad (37)$$

is the composition of the two mappings v and S_t . It is easy to see that v_t is again a state, and that all properties discussed in the previous section that v may possess are inherited by v_t .

Thus we may recast the dynamics in the **Schrödinger picture**, where quantities are fixed and states change with time. The dynamics of the time-dependent states v_t is then given by (37). Of course, in this picture, the dynamics is deterministic, too.

10.2 Examples.

(i) In **classical mechanics**, (34) implies for an ensemble state of the form

$$v_t(f) = \int_{\Omega_{cl}} \rho(\omega, t) f(\omega) d\omega$$

the **Liouville equation**

$$i\hbar \frac{d\rho(t)}{dt} = \{H, \rho(t)\}.$$

(ii) In **nonrelativistic quantum mechanics**, (35) implies for an ensemble state of the form

$$v_t(f) = \text{tr } \rho(t) f$$

the **von Neumann equation**

$$i\hbar \frac{d\rho(t)}{dt} = [H, \rho(t)].$$

(iii) **Bohmian mechanics** has no natural Heisenberg picture, cf. sc Holland [35, footnote p.519]. The reason is that noncommuting position operators at different times are assumed to have sharp values. Thus the results of this section do not apply to it.

In a famous paper, EINSTEIN, PODOLSKY & ROSEN [20] introduced the following criterion for elements of physical reality:

If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity

and postulated that

the following requirement for a complete theory seems to be a necessary one: every element of the physical reality must have a counterpart in the physical theory.

Traditionally, elements of physical reality were thought to have to emerge in a classical framework with hidden variables. However, to embed quantum mechanics in such a framework is impossible under natural hypotheses (KOCHEN & SPECKER [42]); indeed, it amounts to having states in which all Hermitian quantities are sharp, and we have seen that this is impossible for quantum systems involving a Hilbert space of dimension 4 or more.

However, the reference values of states with numerical reference values for *all* Hermitian quantities, and in particular the reference values of ensemble states, are such elements of physical reality: If one knows in a state $v = v_0$ all reference values with certainty at time $t = 0$ then, since the dynamics is deterministic, one knows with certainty the reference values (36) at any time. In this sense, ensemble states provide a realistic interpretation of quantum mechanics.

Taking another look at the form of the Schrödinger dynamics (36), we see that the reference values behave just like the particles in an ideal fluid, propagating independently of each other. We may therefore say that the Schrödinger dynamics describes the **flow of truth** in an objective, deterministic manner. On the other hand, the Schrödinger dynamics is completely silent about *what* is true. Thus, as in mathematics, where all truth is relative to the logical assumptions made (what is considered true at the beginning of an argument), in theoretical physics truth is relative to the initial values assumed (what is considered true at time $t = 0$).

In both cases, theory is about what is consistent, and not about what is real or true. The formalism enables us only to deduce truth from other assumed

truths. But what is regarded as true is outside the formalism, may be quite subjective and may even turn out to be contradictory, depending on the acquired personal habits of self-critical judgment.

What we can possibly know as true are the *laws* of physics, general relationships that appear often enough to see the underlying principle. But concerning *states* (i.e., in practice, boundary conditions) we are doomed to idealized, more or less inaccurate approximations of reality. WIGNER [78, p.5] expressed this by saying, *the laws of nature are all conditional statements and they relate only to a very small part of our knowledge of the world.*

11 Epilogue

The axiomatic foundation given here of the basic principles underlying theoretical physics suggests that, from a formal point of view, the differences between classical physics and quantum physics are only marginal (though in the quantum case, the lack of commutativity requires some care and causes deviations from classical behavior). In both cases, everything flows from the same assumptions simply by changing the realization of the axioms.

It is remarkable that, in the setting of Poisson algebras described and explored in later parts of this series of papers, this remains so even as we go deeper into the details of dynamics and thermodynamics.

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